

Theory of Laser Mechanoluminescence in Coloured Alkali Halid Crystals

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(Received on: July 9, 2013)

ABSTRACT

Luminescence in several non-coloured organic and inorganic crystals by a 20 ns, 1060 nm pulse from a N_d glass laser whose pulse energy varied from 0.5 to 4 J cm⁻² (=200MW peak power). The spectra of laser induced emission were obtained by using a silicon intensified (SIT) Videocon detector and a multichannel analyser. So far as the time dependence of ML in alkali halide crystals is concerned our preliminary observations have shown the occurrence of two ML peaks.. The first peak appears almost in the presence of shock-wave and the second peak appears after the cessation of shock-wave. The decay time of ML intensity after the first and second peak gives the pinning time of dislocations and the lifetime of electrons in the dislocation band, respectively. The ML excited by invisible laser pulses may be an important optical tool to determine the parameters of dislocations in crystals. This needs a further detailed investigation. So far as coloured alkali halide crystals are concluded no theoretical study has been made to date.

Keywords: alkali halide crystals, luminescence, mechanoluminescence, dislocation.

INTRODUCTION

Mechanical deformation of solid is known as mechanoluminescence (ML). It can be excited by cutting, cleaving, compressing or impulsive deformation of solids. So far as the ML excitation is

concerned, the crystals are either deformed slowly at the fixed strain rate or by applying a statistical load on crystals or by impulsive deforming the crystals¹⁻⁴. Recently it has been found that infrared laser pulses produce shock-wave in the solids. Thus ML can be excited by laser pulses instead of direct

deformation of solids. We have been interested whether ML could be made to occur using a high energy laser pulses as the stress inducing agent⁵. The present paper reports the theory of laser ML in colored alkali halide crystals. In analogy with the ML caused by the deformation owing to laser pulses may be called as laser ML. The others materials like elemental and III-V semiconductors exhibit ML during their fracture, which is not related to the movement of dislocations, hence laser ML in colored alkali halide crystals may be observed during only when intense laser shocks pulses instead of direct deformation of solids and laser will create cracks in this semiconductor as such theory of laser ML in colored alkali halide crystals may be quite different from that of II-VI semiconductors whereby intense ML is observed during the direct deformation of solids and the movement of dislocations in these semiconductors.

THEORY

In a crystal having N_d dislocation of unit length per unit volume, if r_F is radius of interaction of dislocation with F-centres and v_d is the average velocity of dislocations, then in unit time, N_d dislocations may interact with the F-centres lying the volume $N_d v_d r_F$. If n_F is the density of F-centres, then for a crystal of unit volume, the rate of interaction of F-centres with dislocations may be given by

$$g_i = N_d v_d r_F n_F = \frac{\dot{\epsilon}}{b} r_F n_F \quad (1)$$

where b is the Burgers vectors and $\dot{\epsilon} = N_d v_d b$, is the strain rate.

Suppose a coloured alkali halide crystal is exposed to a laser pulse whose intensity is given by $I = I_o \exp(-t / \tau_L)$, where I_o is the maximum intensity and τ_L is the duration of a laser pulse. The laser pulse will produce strain in the crystal and the time dependence of strain rate $\dot{\epsilon}$ produced in the crystal may be given by

$$\dot{\epsilon} = A I_o \exp(-t / \tau_L) \quad (2)$$

where A is the correlating factor between g_i and intensity of laser pulse.

Thus from eqs(1) and (2), we get

$$g_i = \frac{A I_o \exp(-t / \tau_L) r_F n_F}{b}$$

$$\text{or} \quad g_i = g_o \exp(-t / \tau_L) \quad (3)$$

$$\text{where } g_o = \frac{A I_o r_F n_F}{b}$$

In the expansion region of dislocations, the average energy E_i of F-centres interacting with dislocations is higher as compared to the non-interacting F-centres⁴. Thus, E_i will be lie between the normal ground state of F-centres and the dislocation band. If α_1 is the rate constant for jumping of interacting F-centres electrons to the dislocation band, and α_2 is the rate constant for the dropping back to the normal F-level, then we can write the following rate equation

$$\begin{aligned} \frac{dn_i}{dt} &= g_i - (\alpha_1 + \alpha_2) n_i \\ &= g_i - \alpha n_i \end{aligned} \quad (4)$$

where $\frac{1}{(\alpha_1 + \alpha_2)} = \tau_L$ is the lifetime of interacting F-centres and n_i is the number of

F-centre electrons at any time t and $\alpha = (\alpha_1 + \alpha_2)$.

from eqs (3) and (4), we get

$$\frac{dn_i}{dt} = g_o \exp(-\alpha_L t) - \alpha n_i \quad (5)$$

$$\text{where } \alpha_L = \frac{1}{\tau_L}$$

eqs (5) may be written as

$$\frac{dn_i}{dt} + \alpha n_i = g_o e^{-\alpha_L t} \quad (6)$$

we get

$$n_i = -\frac{g_o}{(\alpha_L - \alpha)} \left[e^{-\alpha_L t} - e^{-\alpha t} \right] \quad (7)$$

Using eq (7) the rate of generation of electrons in the dislocation band may be written as

$$g = \alpha_i n_i$$

$$\text{or } g = -\frac{\alpha_1 g_o}{(\alpha_L - \alpha)} \left[e^{-\alpha_L t} - e^{-\alpha t} \right] \quad (8)$$

for $\alpha_L \gg \alpha$ eq. (8) may be expressed as

$$g = \frac{\alpha_1 g_o}{\alpha_L} e^{-\alpha t} \quad (9)$$

When the dislocations containing electrons are moving in a crystal, then the electrons may recombine with the defect centers containing holes also with the deep trap present in the crystals. The retrapping of dislocation electrons in the negative ion vacancies may also take place. Suppose N_1 , N_2 and N_3 are densities of recombination centers, deep traps and negative ion vacancies (without trapped electrons), respectively, and σ_1 , σ_2 and σ_3 are the capture cross sections for the recombination centers, deep trap and negative ion vacancies, respectively, then the rate equation may be written as

$$\frac{dn_d}{dt} = g_o e^{-\alpha t} - \sigma_1 N_1 v_d n_d - \sigma_2 N_2 v_d n_d - \sigma_3 N_3 v_d n_d$$

$$\text{or } \frac{dn_d}{dt} = g_o e^{-\alpha t} - n_d / \tau_d$$

$$\text{or } \frac{dn_d}{dt} = g_o e^{-\alpha t} - \alpha_d n_d \quad (10)$$

$$\text{where } \tau_d = \frac{1}{(\sigma_1 N_1 + \sigma_2 N_2 + \sigma_3 N_3)}$$

$$\text{and } \alpha_d = \frac{1}{\tau_d}$$

Equation (12) may be written as

$$\frac{dn_d}{dt} + \alpha_d n_d = g_o e^{-\alpha t} \quad (11)$$

we get

$$n_d = \frac{g_o}{(\alpha_d - \alpha)} \left[e^{-\alpha t} - e^{-\alpha_d t} \right] \quad (12)$$

If η is the probability of radiative recombination, then the deformation induced ML intensity for a crystal of volume V containing N_d dislocations of unit length may be expressed as

$$I = \eta \sigma_1 N_1 v_d n_d$$

$$\text{or } I = \frac{\eta \sigma_1 N_1 v_d A I_o r_F n_F}{b(\alpha_d - \alpha)} \left[e^{-\alpha t} - e^{-\alpha_d t} \right] \quad (13)$$

Equation (13) indicates that I_o should be maximum for a particular value of time t given by

$$t_m = \frac{1}{(\alpha_1 - \alpha)} \ln \left(\frac{\alpha_d}{\alpha} \right) = \frac{1}{(\alpha_L - \alpha)} \ln \left(\frac{\alpha_d}{\alpha} \right) \quad (14)$$

For $\alpha_d t \gg 1$, eq (13) may be expressed as

$$I = \frac{\eta \sigma_1 N_1 v_d A I_o r_F n_F}{b(\alpha_d - \alpha)} e^{-\alpha t} \quad (15)$$

Eqn. (15) shows the exponential decay of ML intensity I , where the decay time will be controlled by α , i.e., the pinning time of dislocations.

It is to be noted that the electrons captured by dislocations have two types of motions, firstly, they move with dislocations, and secondly they also move along the dislocation axis with a very low velocity of the order of 0.1cm/sec. Thus, initially the ML intensity should decay with a fast rate and then it should decay with a slow rate. The first decay time should give the pinning time of dislocations and second lifetime of the electrons in the dislocation band.

CONCLUSIONS

The important conclusions drawn from the present investigation are as given below :

- (i) When the ML in a coloured alkali halide crystals is excited by the deformation caused by a laser pulse, then the ML intensity versus time curve should possess two peaks, where the first peak should occur in the region where deformation takes place owing to laser

pulse and the second peak should occur in the post-deformation region.

- (ii) In the laser-stimulated ML in coloured alkali halide crystals, the ML intensity should decay with a fast rate and then it should decay with a slow rate. The first decay time should give the pinning time of dislocations and second lifetime of the electrons in the dislocation band.
- (iii) By using laser pulse and an optical fiber, the ML may be observed owing to the movement of a single dislocation in coloured alkali halide crystals.

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